Supplementary Information to accompany

Electronic Excitation to Singlet States of 1,3-C_4F_6, c-C_4F_6 and 2-C_4F_6 by Electron Impact - Electron Energy-Loss Spectroscopy and *Ab Initio* Calculations

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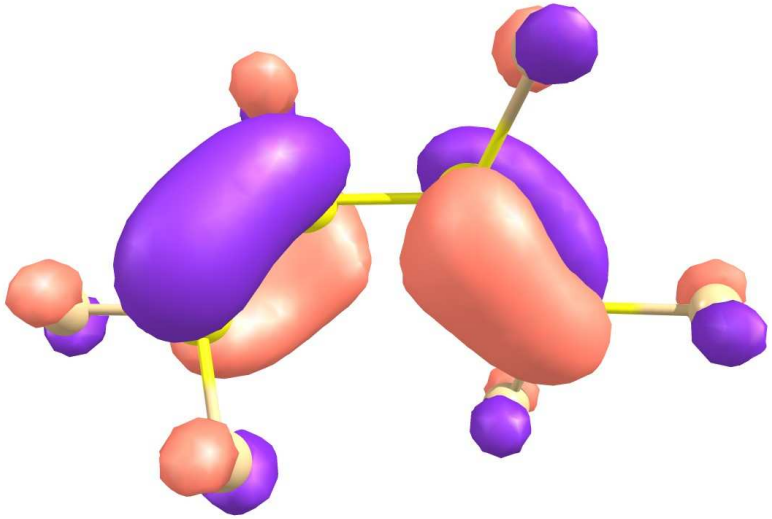
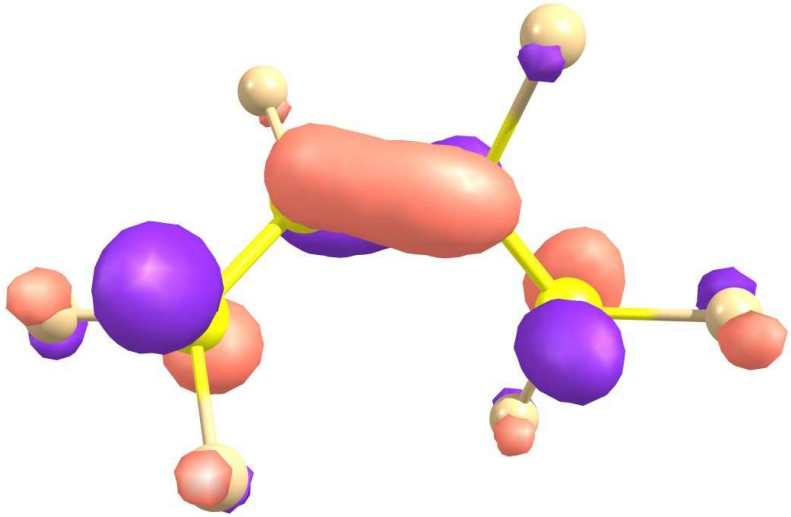
Molecular orbitals and lowest Rydberg states

The set of figures show the highest occupied molecular orbital (HOMO), lowest unoccupied molecular orbital (LUMO), second highest occupied molecular orbital (SHOMO) and second lowest unoccupied molecular orbital (LUMO+1) of C_4F_6 isomers, hexafluoro-1,3-butadiene (1,3-C_4F_6), hexafluorocyclobutene (c-C_4F_6) and hexafluoro-2-butyne (2-C_4F_6). Additionally, the Lowest Rydberg states for the D_{3d} isomer, hexafluoro-2-butyne (2-C_4F_6) are shown.

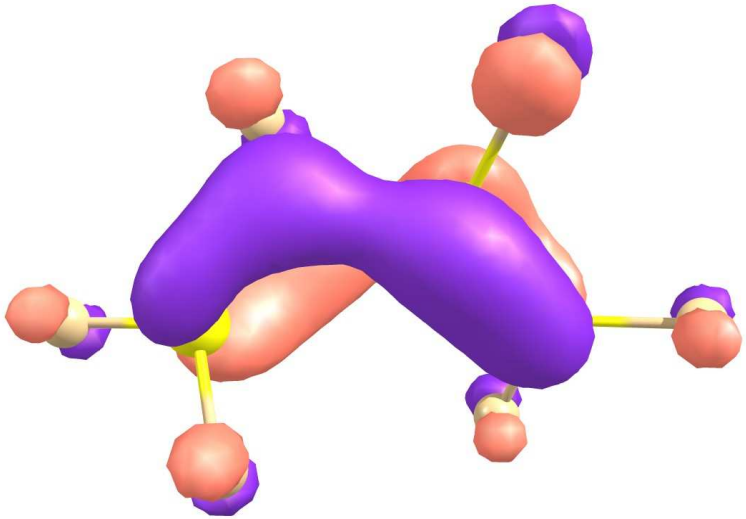
Figure Ia) – molecular orbitals of hexafluoro-1,3-butadiene (1,3-C_4F_6)



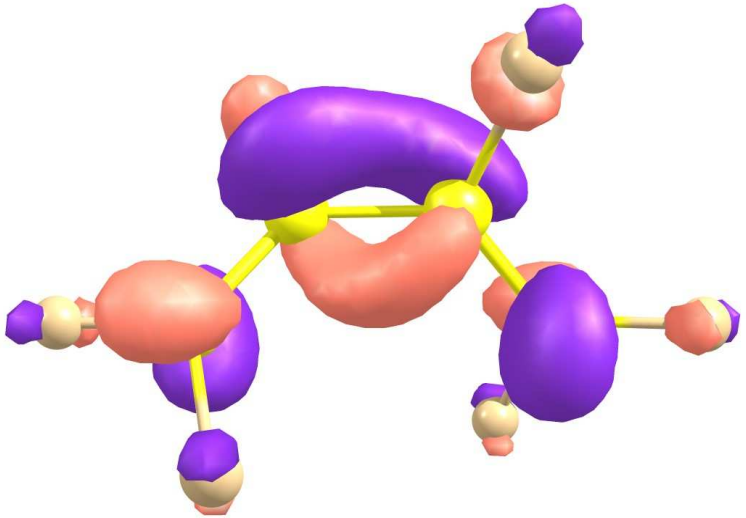
HOMO 20a π_a



LUMO 20b π^*_b

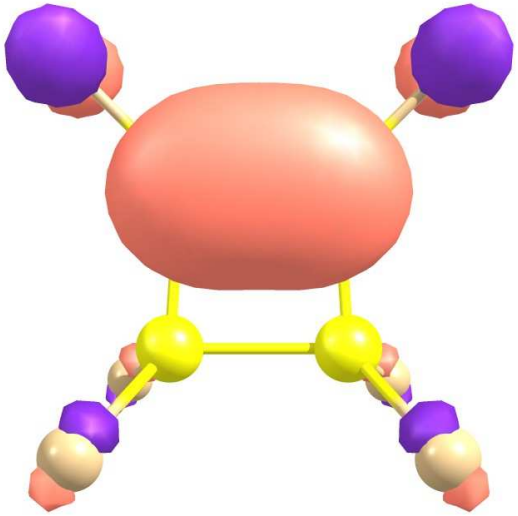


SHOMO 19b π_b

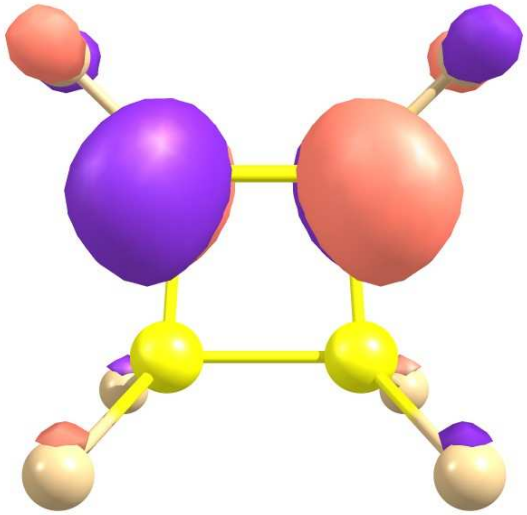


LUMO+1 21a π^*_a

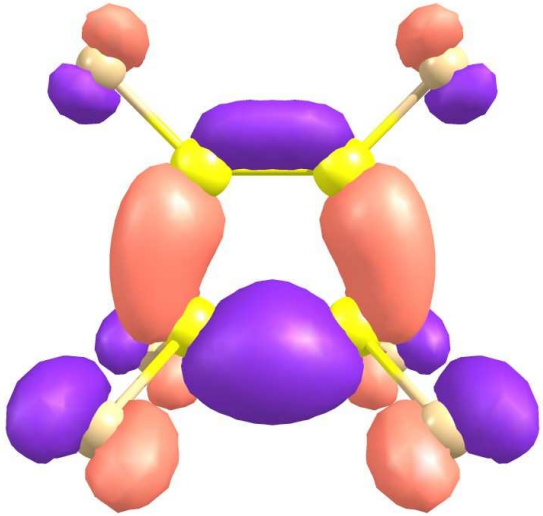
Figure Ib) – molecular orbitals of hexafluorocyclobutene (c-C_4F_6)



HOMO $7b_1$

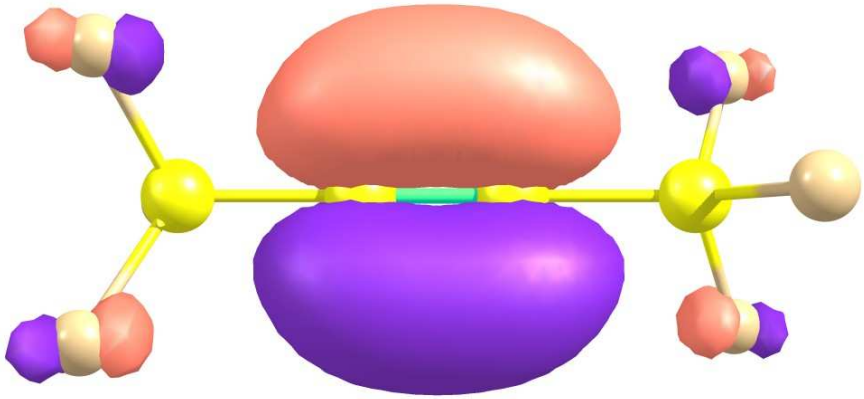


LUMO $1a_2$

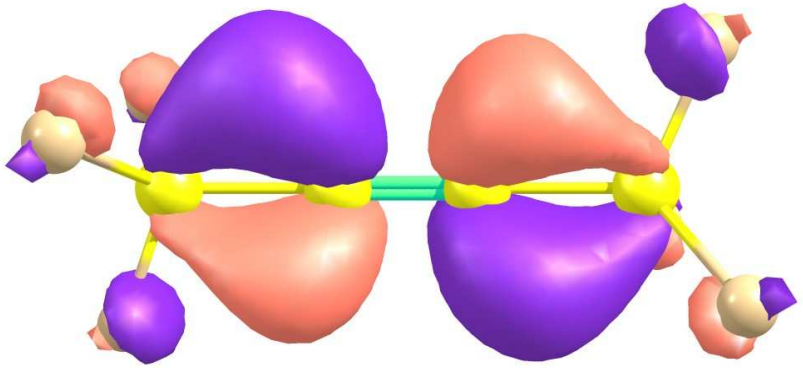


SHOMO $14a_1$

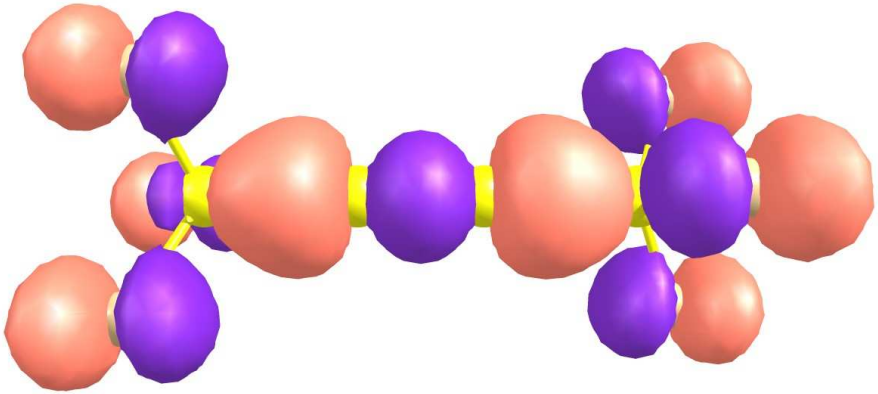
Figure Ic) – molecular orbitals of hexafluoro-2-butyne (2-C_4F_6)



HOMO ($6e_u$ or $13b_u + 7a_u$)

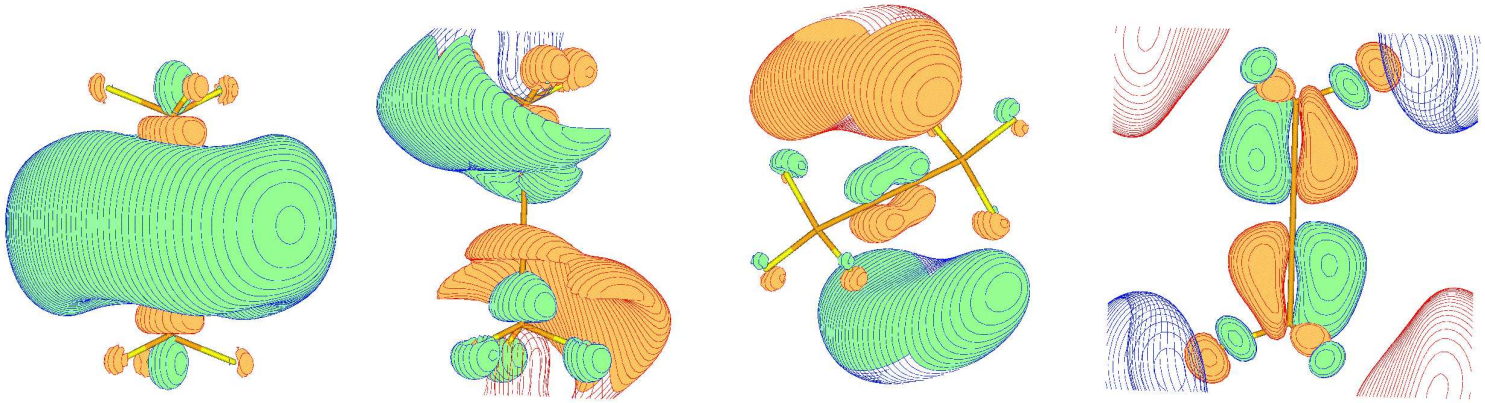


LUMO ($6e_g$ or $7b_g + 14a_g$)



SHOMO ($1a_{2g}$ or $6b_g$)

Figure II – Lowest Rydberg states for the D_{3d} isomer, hexafluoro-2-butyne (2-C_4F_6)



3sσ 3pσ 3pπ 3dπ